2,3,4-Trimethylpentane
565-75-3 | DTXSID6060343

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 275 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.36e-01

Confidence level: 6.06e-01

Nearest Neighbors from the Training Set

Image not found

Propylbenzene
Measured: 741
Predicted: 859

Image not found

Ethylbenzene
Measured: 170
Predicted: 271

Image not found

1,3,5-Trimethylbenzene
Measured: 661
Predicted: 493

Image not found

1,2,3-Trimethylbenzene
Measured: 631
Predicted: 691

Image not found

Isophorone
Measured: 25.1
Predicted: 103